# LDRD

**Laboratory Directed Research and**
**Development at the National Laboratories**

# Highlights

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**U.S. DEPARTMENT OF ENERGY**

# Contents
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Energy systems studied by DOE LDRD researchers, from astronomical to planetary to environmental to nanolevel and biological (bio-nano) to quantum levels of organization.

# Laboratory Directed Research and Development:

## *The Department of Energy's Engine of Discovery*

Over the past century, the pace of scientific discovery has accelerated more quickly than at any time in human history, and we are the beneficiaries. Diseases that plagued our great grandparents are now footnotes in history. Theoretical and technological advances that helped win wars and protect our freedom are today powering our cities and helping to remediate our environment. Boundaries that once seemed impossible are forming the basis of a new American economy.

To meet the Nation's key challenges, the Atomic Energy Act of 1954 provided the basis for DOE national laboratories to respond immediately to developments at the cutting-edge of science and technology while retaining the best scientific and technological minds. To help re-energize this commitment to national laboratory scientific, technological, and engineering excellence, in 1991 the U.S. Congress authorized them to devote a relatively small portion of their research effort to creative and innovative work that serves to maintain their vitality in science and technology (S&T) disciplines relevant to DOE and national security missions. Since then, this effort has been formally called Laboratory Directed Research and Development (LDRD).

Today, national laboratory LDRD scientists are pursuing high-risk, high-value science and engineering research that addresses DOE's key challenges in securing a sustainable energy future, improving nuclear and environmental security, and promoting U.S. leadership in scientific discovery and innovation. From tiny sensors that guard against nuclear materials proliferation to novel properties of matter in the nanoworld to renewable and carbon-neutral energy sources—and the computational expertise to support all these research arenas—LDRD provides national laboratories the opportunity to maintain and advance state-of-the-art science and technology capabilities for laboratory scientists' most innovative and promising research ideas.

This publication offers a small sampling of LDRD research highlights from across DOE national laboratories. LDRD research is an essential component in DOE's charge to sustain and broaden world-class science and engineering capabilities within the national laboratories, and to sustain—now and into the future—the science and engineering preeminence of the United States.
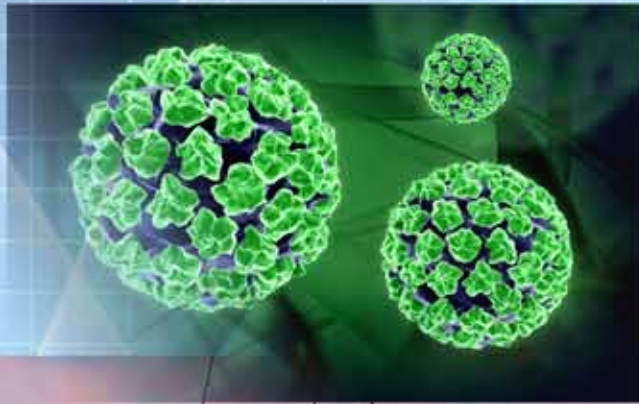
# Energy Security

LDRD efforts in energy security span a broad vista, all directed at leading the way toward a transformation in the ways that we produce, conserve, and utilize energy. The challenges driving these efforts include the reduction of our dependence on foreign fossil-fuel and of our production of greenhouse gases. More-efficient, lower-emission internal combustion engines are required in the short term. In the longer term, to achieve the nation's 2035 goal of generating 80% of our electricity from clean energy sources, national laboratory LDRD programs must assist this transition with improved clean technologies, such as more-effective wind turbines, and more-efficient photovoltaic and solar-thermal technologies. Implicit in this challenge are both modeling and experimental research projects to address the modernization of the electric grid, and breakthroughs for more-efficient—even loss-less—current transmission. Another key aspect is reduced energy consumption through increased efficiency of electricity-consuming devices, such as appliances and lighting fixtures. National laboratory LDRD projects are researching novel materials and solutions leading to improved-efficiency and cost-effective solid state lighting.

Reducing greenhouse gas emissions and consuming less fossil fuel requires multiple technological advances in vehicular transportation. Novel battery concepts for hybrid-electric vehicles, in the context of both existing materials such as lithium and of potential surrogate materials is an LDRD focus. Another is research into a variety of routes to efficient biofuels. There is also the prospect of a hydrogen-based transportation economy, with challenges from fuel cells to hydrogen storage. In addition, there are initiatives seeking to directly recycle waste carbon dioxide from fossil fuel combustion to produce synthetic transportation fuels utilizing sunlight energy.

Typifying LDRD projects, these highlights represent preliminary, seminal research into technological challenges of great interest in current DOE programs.

# Unlocking the Mysteries of Super Current Carriers

## Layer-by-layer synthesis method allows studies of materials and mechanisms enabling high-temperature superconductivity
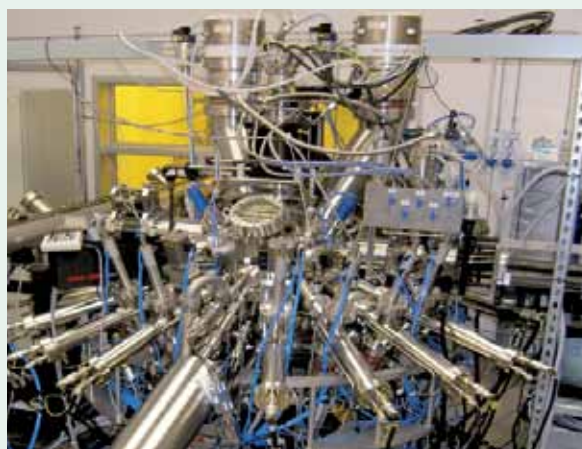
Scientists at Brookhaven National Laboratory have developed a unique system for synthesizing single atomic layers of high-temperature superconductors—materials carrying current with no energy loss when cooled below a certain temperature. Thin films, multilayers and superlattices made with this method are enabling experiments that probe the basic physics of high-temperature superconductivity. The challenge is to figure out how to raise the temperature at which the materials operate. "The ultimate goal for scientists is to create superconducting materials with transition temperatures as high as possible — above room temperature if at all possible," said Brookhaven physicist Ivan Bozovic.



**The atomic-layer-by-layer molecular beam epitaxy system at BNL.**

## Why It Matters

Experimental results could lead to the design of materials that transform the U.S. energy landscape with applications such as zero-loss power transmission lines and improved energy storage systems. Superconducting power lines alone could improve the power-carrying capacity of the U.S. electrical grid fivefold and save $120 billion per year.

Thin film superconductors may also lead to devices with "tunable" superconductivity — an effect that can be turned on or off by external controls, for use in devices such as superconductive transistors, and eventually, in ultrafast, power-saving electronics.

"Electronic devices already consume a large fraction of our electricity usage—and this segment is growing fast." Bozovic said. "Clearly, we will need less-power hungry electronics in the future."

## Methods

By building superconducting materials one atomically perfect layer at a time using a unique Brookhaven-developed molecular beam epitaxy system, Bozovic and his collaborators have been able to conclude the following.

- A single copper-oxide layer doped with charge-carriers can sustain high-temperature superconductivity.
- Two-layer thin films where neither layer is itself superconducting can exhibit a nanometer-thick region of superconductivity at their interface, even at temperatures above those achievable with single-layer superconductors.
- In a single copper-oxide layer without doping, quantum spin liquid forms. In this exotic state of matter, the orientation of electron magnetic

moments, or "spins," fluctuates rapidly in a correlated manner.

- When an electron moves inside a copper-oxygen plane, it interacts strongly with ions in neighboring layers, and triggers their vibrations; this strong interaction is probably an important puzzle piece /[of high-temperature superconductivity.

- A thick barrier of superconductor with a low critical temperature can transmit supercurrent at a temperature four times higher, if sandwiched between two strong superconductors; this Giant Proximity Effect affects the entire barrier layer.

- Fleeting fluctuations in superconductivity disappear just above the temperature at which superconductivity sets in, indicating that a loss of coherence among electron pairs "turns off" the superconductivity.

## What's Next

Brookhaven researchers will continue to gain a better understanding of high-temperature superconductivity and attempt to synthesize novel, superior superconducting metamaterials. Bozovic's layer-by-layer synthesis method and ability to strategically alter an individual layer's composition might also be used to explore and possibly control other electronic phenomena that emerge at the interfaces between layered materials.

## Publications

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I. Bozovic et al., *Phys. Rev. Letters*, vol. 89, p. 107001, 2002; A. Gozar et al., *Nature*, vol. 455, p. 782, 2008; S. Smadici et al., *Phys. Rev. Letters*, vol.102, p. 107004, 2009.

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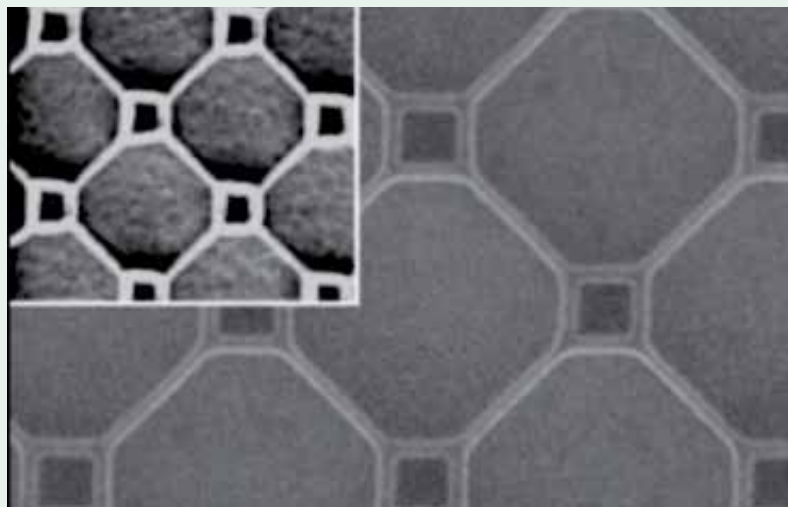


**Fragment of superconducting thin film patterned with 25 nm nanowire to yield nanoloops of 150 and 500 nm.**

## *"We will need less-power hungry electronics in the future."*

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## Acknowledgements

# Holistic Approach to Energy-efficient Computing Architecture

*LBNL researchers have proposed an innovative approach to overcome the energy demands and performance limitations of conventional supercomputers by using low-power embedded microprocessors*

The potential energy demands for exascale computing facilities are expected to increase to an unsustainable level. Historically, supercomputer makers build larger and more powerful systems by increasing the number of conventional microprocessors—usually the same kinds used to build personal computers. However, continuing this approach for exascale computing will be profoundly impractical because power requirements are projected to exceed 200 megawatts, enough energy to power a city of 200,000 residents.
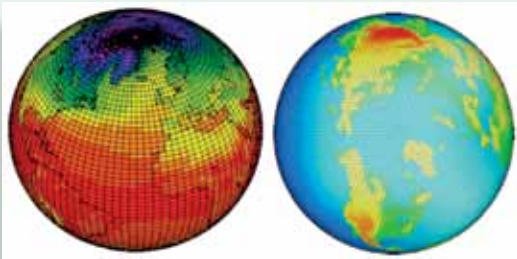


**Reformulating the computational mesh for the climate model.**

This project's purpose is the development of fundamental advances in energy-efficient computational science. It involves taking a vertical slice through the space of applications, algorithms, software, and hardware (to examine a representative sample) to study how to build the most energy-efficient system to solve a computation science problem. The initial target was climate simulation, and the energy-efficient solution is likely to require higher degrees of parallelism in climate algorithms and software, as well as new hardware designs based on technology from outside the traditional workstation and server domains. The intended result was a proof-of-concept machine design, with supporting analyses, and new algorithms and software techniques.
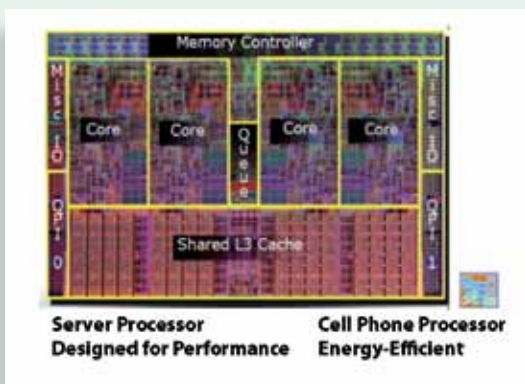


**Simpler design of embedded processors consumes less chip area so hundreds can be used per chip, delivering 10× the performance for 1/10th the power.**

## Why It Matters

High-end simulation and modeling that is enabled by exascale computing will have a transformative impact on numerous national and global problems. On the other hand, the energy demands for such exascale computing would increase at an unsustainable level. Therefore, dramatic improvements over current technologies in efficient computing are essential to enable the projected computational requirements. The Berkeley team proposed a new approach to high performance computing system design that encompasses hardware, software, and algorithms—enabling a 100 times improvement in computational efficiency over current technologies.

In order to develop fundamental advances, the team applied a unique approach to a climate simulation problem where the solution required higher degrees of parallelism in the climate algorithms, as well as new hardware designs based on technology from outside traditional workstation and server

domains, particularly low-power embedded technology. The successful outcome was a proof-of-concept machine design, along with supporting analyses of how this compares to alternative designs, and new algorithms and software techniques, as needed, to make the case for feasibility of computing the science problem on the system.

## Methods

The researchers studied several different formulations of the global climate model to further refine projected computational requirements, including extrapolations of the Community Atmospheric Model (CAM), developed at the National Center for Atmospheric Research in Boulder, Colorado, and a family of Global Cloud Resolving Climate Model (GCRM) models developed by David Randall's group at Colorado State University (CSU). The LBNL researchers collaborated with CSU to successfully demonstrate the concept by building a prototype system to run the CSU icosahedral GCRM model.

The team developed an energy-efficient hardware design based on low- power embedded technologies with architecture extensions tailored to the requirements of the target application, then ran the full climate model on a cycle-accurate simulation of the full node design to demonstrate that Green Flash was nearly 80 times more energy efficient per watt than a conventional high-performance computing solution. The team used auto-tuning to optimize the performance of the code for the Green Flash hardware, using the computer to search through a large number of code transformations. The team also created a co-tuning process that combined the search of hardware design options with auto-tuning of the software model to find an additional four-times improvement in energy efficiency over traditional hardware design techniques.

*" exascale power requirements  projected to exceed . . . energy to power a city of 200,000"*

## What's Next

The tools developed for this project will address the transformational impacts on high-end computing required for future exascale computing science problems. This project raised awareness of the importance of CoDesign in developing cost-effective and energy-efficient computing for the emerging DOE exascale program. CoDesign now plays a central role in the DOE Exascale program with the recent establishment of CoDesign centers. The recently funded CoDEx (CoDesign for exascale) project at LBNL has taken the tools developed in this project to develop efficient high-performance architectures for other mission-critical DOE exascale program applications.

## Publications

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M. Wehner, L. Oliker, and J. Shalf, "Green Flash: Designing an energy efficient climate supercomputer," *IEEE Spectrum*, 2009.

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"Green Flash" webpage: http://www.lbl.gov/CS/html/green-flash.html.

## Acknowledgements:

# Potential New Method for Hydrogen Production and Fuel Cell Processes

## Carbon nanotube-hydrogenase technology produces hydrogen while saving precious metals
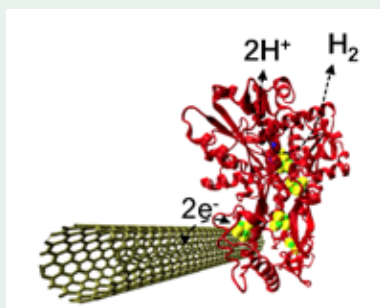


**Drawing of a model of an SWNT-hydrogenase complex illustrating the reduction of hydrogen ions from water into molecular hydrogen.**

One of the significant challenges in developing scalable technologies for a hydrogen economy is to reduce the need for platinum and other precious metal catalysts that render chemical processes faster and more efficient. These catalysts are necessary to achieve water-splitting to make hydrogen (and oxygen), and for fuel cells to convert the chemical energy of hydrogen reactions into electricity. In this project, substitute catalytic compounds are being devised through the combination of bio-inorganic catalysts (in the form of biological enzymes) and materials chemistry (in the form of carbon nanotubes).

NREL's dual-focus research with carbon nanotube technology and also in developing scalable expression of enzymes constitutes a huge step toward minimizing the use of these precious metals and improving hydrogen production.

## Why It Matters

NREL's research demonstrated that when certain biocatalysts (enzymes that naturally function in the production or use of hydrogen—generally known as hydrogenases and present in many different organisms) were combined with single-wall carbon nanotube (SWNT) films, the catalytic performances matched those of platinum. While this precious metal is in limited supply, biocatalysts and carbon nanotubes, composed of earth-abundant elements (carbon, oxygen, nitrogen, sulfur, and iron), are more available. "This technology shows the potential to achieve high catalytic performances from more-common materials," said Paul King, principal investigator on the project. "The SWNT films developed and used during this research also have the potential to improve performances of other catalytic (and biocatalytic) materials that convert carbon dioxide into carbon-based fuels," noted Drazenka Svedruzic, a co-investigator.

## Methods

NREL developed and tested ways to apply SWNT suspensions as films (made by filtration, air-brush or ultrasonic spraying, drop-casting) to different substrates (indium tin oxide or ITO, fluorine-doped tin oxide or FTO, carbon-cloth, pyrolytic graphite, glassy carbon). Single-wall carbon nanotube suspensions are composed of two basic SWNT types — metallic

and semiconducting — which were separated using a preparative technique developed by Jeffrey Blackburn of NREL. Ultrasonic spraying (first developed by Rob Tenent of NREL for preparation of transparent conducting electrodes) and subsequent nitric acid treatment produced the most stable and reproducible films, with carbon-cloth being the best substrate. These films showed improved hydrogenase electrocatalytic activity.

Researchers used the film-preparation technique to test the effect of different SWNT compositions (metallic or semiconducting) as the electrode material, then identified and characterized how the hydrogenase electrocatalytic behavior responded. They found that the metallic fraction of SWNTs performed the best for this application.

## What's Next

This work by NREL researchers is a pioneering effort that demonstrates the effect of carbon nanotube electronic structure on the performance of an enzyme-based electrode. These electrodes may lead to fabrication of highly electroactive, low-cost, noble-metal-free catalytic electrodes for renewable hydrogen conversion devices.

## Publications

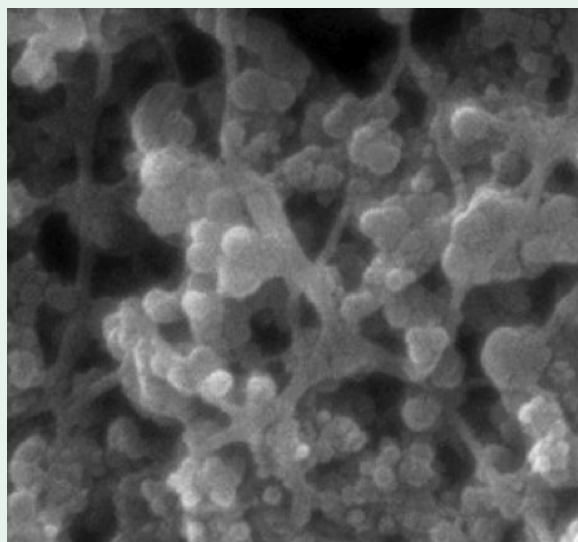McDonald et al., *Nano Letters*, vol. 7(11), pp. 3528–3534, 2007.

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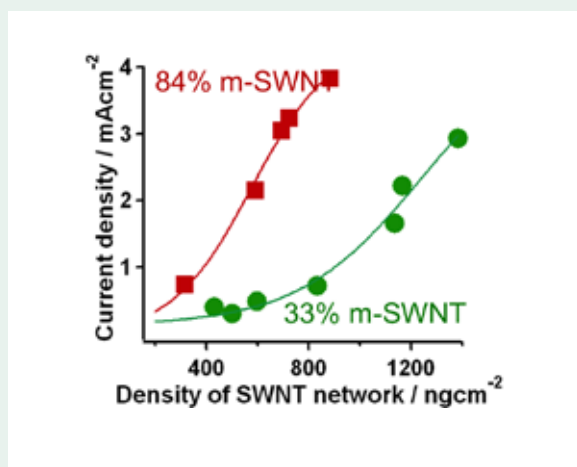Svedruzic et al,, *Journal of the American Chemical Society*, submitted.
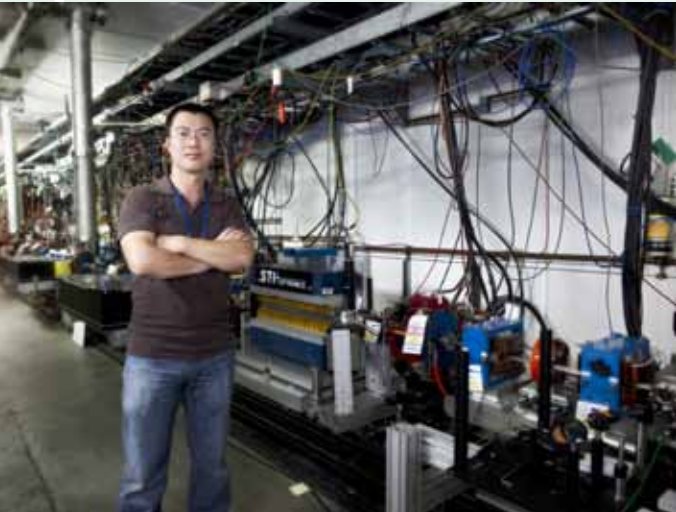
## Acknowledgements

**Scanning electron micrograph (SEM)of a single wall carbon nanotube (SWNT) film.**



**Graph of the improved hydrogen production activities observed with films made from high (red) versus low (green) metallic SWNT contents.**

*" . . . the potential to achieve high catalytic performances from more-common materials."*

**SLAC accelerator physicist Dao Xiang in the NLC Test Accelerator facility at SLAC, where Xiang and his colleagues undertook the Echo 7 experiment** *(Photo by Brad Plummer).*

*"This is an important step; we have demonstrated that EEHG works."*

# Echoes of Future X-ray Laser Technology

### *Spatially and temporally coherent deep-ultraviolet lasers*

Even as scientists are revealing the first, unprecedented images of proteins and viruses from the world's first hard x-ray laser, the Linac Coherent Light Source (LCLS), SLAC researchers are developing the technology for the next-generation facility. In the September 10, 2010 *Physical Review Letters*, the "Echo 7" team described their success at adding an additional, elusive property to x-ray laser beams: temporal coherence. The Echo-7 experiment took infrared laser light and transformed it into deep ultraviolet laser light with both spatial and temporal coherence.

## Why It Matters

Free-electron lasers like the LCLS provide an ultrabright, ultrafast source of x-rays that can be used to probe and characterize properties of materials for energy, computing, biomedical science, and much more, providing images of unprecedented clarity, in part, because they create x-rays that are spatially coherent; in other words, the crests and troughs of individual light waves line up with one another at any given moment, traveling forward in perfect synchrony. With temporally coherent light, the peaks and valleys at one moment match the peaks and valleys a certain amount of time later. A temporally coherent laser beam would give lightsource users an x-ray beam with exquisitely nuanced control for precise imaging of detail near atomic scales and ultrafast processes, showing chemistry in action.

## Methods

The experiments were based on a theory called Echo-Enabled Harmonic Generation (EEHG) proposed by SLAC accelerator theorist Gennady Stupakov. In EEHG, an electron beam interacts with a "seed" laser that already has temporal and spatial coherence, albeit with a longer wavelength than the researchers ultimately need. Interaction with the seed laser causes the electrons in the beam to pack into bunches in just the right pattern to later generate temporally and spatially coherent shorter-wavelength x-ray light.

The LCLS, in comparison, begins not with a seed laser but with random noise, which, in its interaction with the electron

beam, leads to spatially coherent (but not temporally coherent) light. Subsequently, through controlled injection of energy at the Next Linear Collider Test Accelerator, this light is rendered temporally coherent, as well, and is also shortened in wavelength by a factor of four, thereby creating spatiotemporally coherent light of an ultraviolet wavelength.

Eventually, the team would like to decrease the wavelength to 20 percent that size, creating spatially and temporally coherent extreme ultraviolet light that is stable in space and consistent in time.

"This is an important step," said SLAC accelerator physicist Dao Xiang. "We have demonstrated that EEHG works."
This technique is expected to enhance the performance of planned and future free-electron lasers, increasing the temporal control of the beam and reducing the length of the undulator used to generate x-rays from accelerated electrons.
"This experiment was very impressive in terms of both the physics that was measured as well as the speed with which the team put it together," said Accelerator Research Division Director and experiment principal investigator Tor Raubenheimer.

## What's Next
The team is now working to further validate the theory and create shorter wavelengths of temporally coherent light. In the near future, the researchers want to confirm that this technique could be scaled to the x-ray range.

If future experiments are as successful as this one, EEHG may also be used in the proposed LCLS-II facility, to generate fully coherent x-rays that arrive so regularly that they can be synchronized with a laser for pump-probe experiments. With fully coherent x-ray light, researchers at the LCLS could conduct many more challenging ultrahigh-resolution microscopy and imaging studies—valuable additions to an already valuable machine.
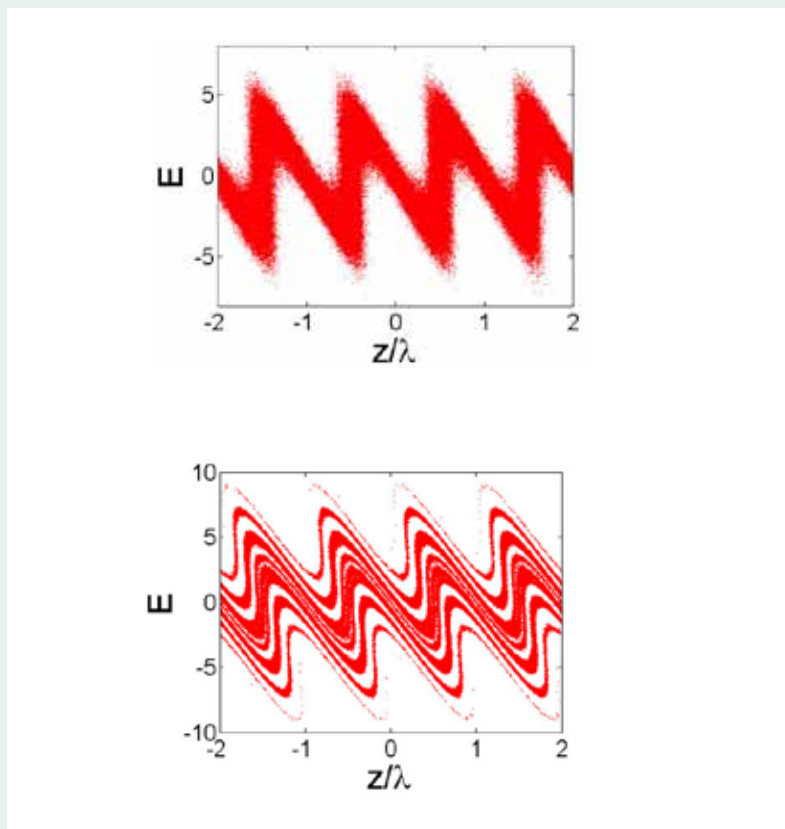


**Top: Infrared laser light; Bottom: Deep ultraviolet laser light with both spatial and temporal coherence.**
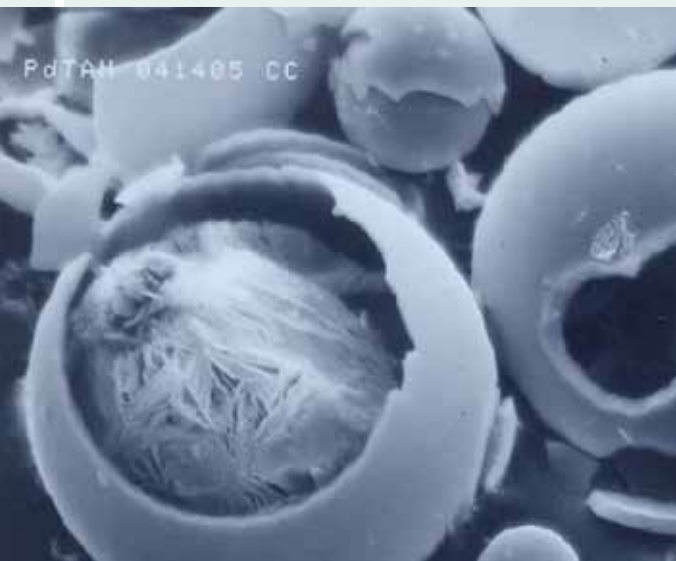
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Demonstration of the Echo-Enabled Harmonic Generation Technique for Short-Wavelength Seeded Free Electron Lasers, *Phys. Rev. Lett.*, vol. 105, p. 114801, 2010 [http://prl.aps.org/abstract/PRL/v105/i11/e114801] .

## Acknowledgements

**Scanning electron micrograph of hollow glass microsphere, with its top removed to show its contents**

*"a protective . . . cocoon for their contents"*

# Porous Wall
# Hollow Glass Microspheres

## *Tiny Glass Spheres for Energy Storage, Medical Applications and Other Uses*

Researchers at Savannah River National Laboratory (SRNL) have developed a new class of materials, dubbed porous wall hollow glass microspheres (PWHGMs).  These miniature balloon-like structures are capable of containing and releasing a variety of materials, with exciting potential for use in areas that range from energy to biomedicine. PWHGMs have a diameter of about half the width of an average human hair (about 50 micrometers). Their walls are only about 1 to 2 microns thick, and contain interconnected pore-channels. These channels can be used to fill the microballoons with special absorbents and other materials of interest—gases, liquids and solids.  For example, initial work centered on using the microspheres to store and release hydrogen gas in controlled fashion, with applications in hydrogen fuel cell automotive technology.

## Why It Matters
What makes SRNL's microspheres unique, and gives them the capability to be useful in so many fields, is the network of interconnected pores in the thin outer shells that allow the tiny "microballoons" to be filled with a diversity of materials for a broad range of applications.  The capability to control pore size in the walls of these unique microspheres gives them exciting potential for use in areas including energy, environmental remediation, drug delivery, hydrogen storage and many other uses. For example, patients who required controlled release of a drug over time might readily benefit from  this technology.  Because the glass spheres provide a protective environment, or cocoon, for their contents, they can also be used to hold reactive or flammable absorbents or stored materials.  This endows them with the potential to provide a safe method of handling, storing or transporting a variety of difficult materials.

## Methods
A glass composition that is chemically disposed to undergo amorphous phase separation is used to produce a hollow glass microsphere.  The microsphere is heat-treated to develop the interconnected microstructure, then subjected to a leaching

process, which results in a sponge-like network structure consisting mainly of silica. Two LDRD projects have had an impact in development and understanding of this unique material. One focused on the impact of composition and temperature on pore size, showing, among other results, that heat treatment temperature, rather than composition was most effective in changing porosity. Heat treatment at 600 °C for 8 hours increased the pore diameter ten-fold, from approximately 100 Å to approximately 1000 Å. A second LDRD project in collaboration with Virginia Polytechnic Institute and Boston University examined chemical and mechanical means of releasing "payloads" contained within the microballoons.
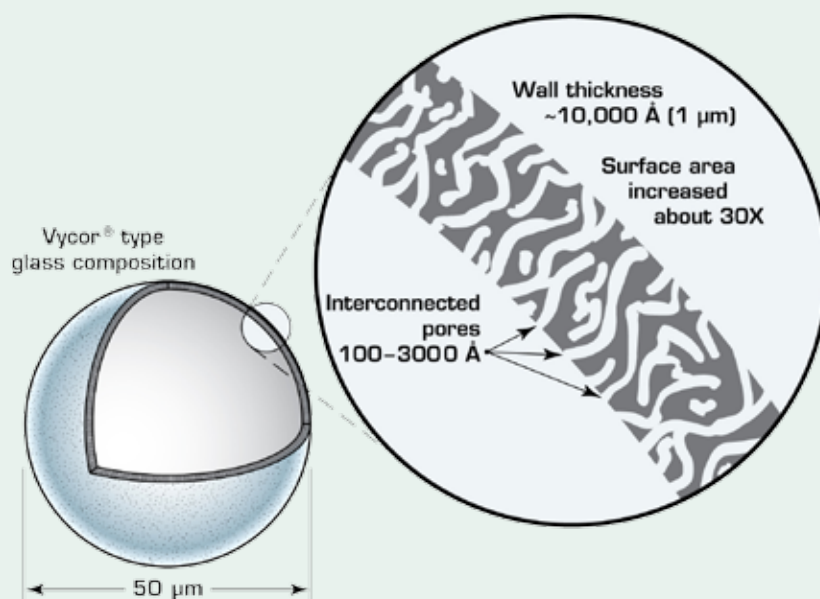


**Schematic of PWHGM, showing porosity of walls**

## What's Next

One patent has been issued with four more pending. The technology has been licensed to a specialty glass manufacturer for developing capabilities for large-scale production. Technology transfer initiatives related to the PWHGMs earned an Honorable Mention in the 2010 Federal Laboratory Consortium Excellence in Technology Transfer Awards.

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R. Mohtadi, K. Tange, T. Matsunaga, G. Wicks, K. Heung, and R. Schumacher, "A New Way for Storing Reactive Complex Hydrides on Board of Automobiles," in Materials Innovations in an Emerging Hydrogen Economy," *Ceramic Transactions*, vol. 202, pp. 91-96, 2009.

K. Heung, G. Wicks, and R. Schumacher, "Encapsulation of Palladium in Porous Wall Hollow Glass Microspheres," *Ceramic Transactions*, vol. 202, pp. 143-148, 2009.

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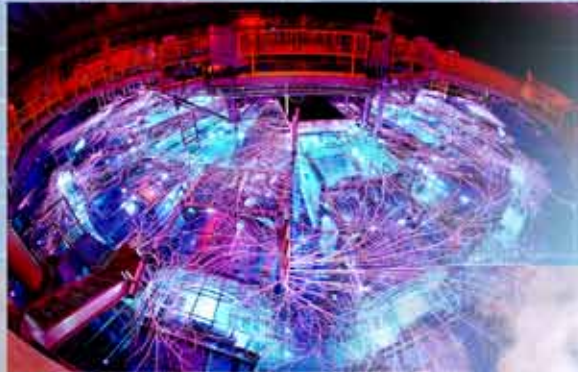
# Nuclear Security

LDRD efforts in support of the DOE's nuclear security mission encompass a range of projects from national defense through environmental defense, beginning with the U.S. nuclear arsenal and the life extension initiatives designed to ensure its functionality for decades to come. Moreover, given the ongoing moratorium on the actual testing of nuclear weapons, engineers must rely on computational simulation, and therefore must ensure that computer models provide an accurate picture of performance, a truly daunting task. LDRD research supports these initiatives, as well as extending its reach into nuclear energy, with projects such as those to attempt to improve both civilian and military nuclear reactor efficiency and functionality, and also to close the nuclear fuel cycle, a key approach to dealing with the problem of spent reactor fuel.

Another important contribution of LDRD research is found in the area of nonproliferation and prevention of nuclear terrorism, attempting to ensure that actinides are not diverted into the hands of non-state actors. Clever advancements in forensics and intelligence analysis are exemplary. A parallel set of R&D activities to which LDRD research efforts contribute is environmental remediation of legacy radiological sites deriving from both weapons and reactor activities.

# Safety-first Next-generation Nuclear Power

## INL collaborative researchers advance foundation for next-generation safety analysis codes

This project is developing the scientific basis and computational technology for a Next-generation Safety Analysis Code (NGSAC) for nuclear power plant safety margin quantification. Led by PI and INL Laboratory Fellow, Nam Dinh, it brings together a multidisciplinary team from INL and collaborators.

The project builds on INL's knowledge base, advanced computational methods, and the emerging formulation of risk-informed safety margin characterization (RISMC). RISMC brings together the methods of deterministic/mechanistic safety analysis and probabilistic risk analysis (PRA) for an integrated risk model. PRA-based risk insights help focus the analysis on risk-significant transients and postulated accidents. Methods of sensitivity analysis (SA) and uncertainty quantification (UQ) incorporated into the R7 code will enable a quantitative phenomena identification and ranking table process to effectively guide the R&D toward uncertainty reduction and render robustness and predictability in safety-issue resolution and plant licensing.

## Why It Matters

As the current fleet of nuclear power plants ages, their continued safe and economic operation would benefit from advanced modeling and simulation capabilities providing improved characterization of safety margins. More than 450 reactors operate worldwide, and many more are planned or under construction internationally. This research may well contribute to safety design and operation of advanced nuclear power plants. The methods in this project provided technical insights that facilitated R&D

planning for the DOE's Light Water Reactor (LWR) Sustainability Program's RISMC pathway.

## Methods

Differing from other national and international efforts to advance reactor simulation, this project exercises a multi-pronged approach, concurrently advancing a novel analysis framework (RISMC), a computational engine, and a verification and validation (V&V) infrastructure.

"This project enabled us to formulate a basic concept of a next-generation safety analysis code as a computational engine for risk-informed safety margin characterization, and to identify both critical capability gaps and high-risk/high-reward developments," Dinh said. "Then we were able to take these findings, investigate them, and make advances that significantly strengthen the technical basis for the development, demonstration, and validation of next-generation system safety codes."

The project focuses on basic capabilities, including fluid flow homogenization, adaptive model refinement, high-order-accurate solution scheme, sensitivity analysis and uncertainty quantification techniques specific to "system analysis," experimental V&V database. Collaborations are ongoing with North Carolina State University (NCSU), Utah State University (USU), and the University of California-Davis (UC-D). For example, published research in high-order-accurate numerical methods in all-Mach compressible flow is performed by Dr. Nourgaliev in collaboration with NCSU's Professor Hong Luo.

## What's Next

In 2010, the LWR Sustainability Program supported development of a β-version of R7 code, which is a prototype NGSAC aimed at plant life extension decision-making. DOE's Nuclear Energy Advanced Modeling and Simulation (NEAMS) program supported implementation and testing of advanced methods in code V&V and uncertainty quantification in R7, and DOE's Consortium for Advanced Simulation of LWRs selected the R7 code as the advanced system simulation engine to be integrated into its VERA package. The V&V database has evolved into a Nuclear Energy Computational Applications Management System that is supported by several DOE-NE Programs. Recognizing the potential role of NGSAC in utility's deliberation in extending LWR plant life beyond sixty years, nuclear experts are participating, with support of the Electric Power Research Institute.

## Selected Publications

Include nine conference papers and three journal publications. A paper on PIV uncertainty led by a USU student won the American Society of Mechanical Engineer's Knapp Award for outstanding original paper in fluid engineering. In addition, the project researchers shared their developments during the 2009 and 2010 Modeling Experimentation Validation (MeV) Summer School, training nearly 100 young researchers and engineers in the field. Dinh is the school's academic dean.

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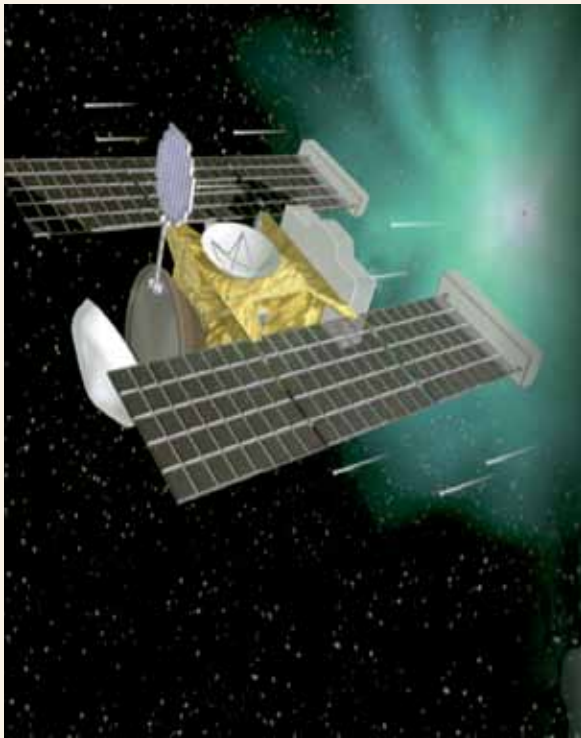
*"validation of next-generation safety codes."*
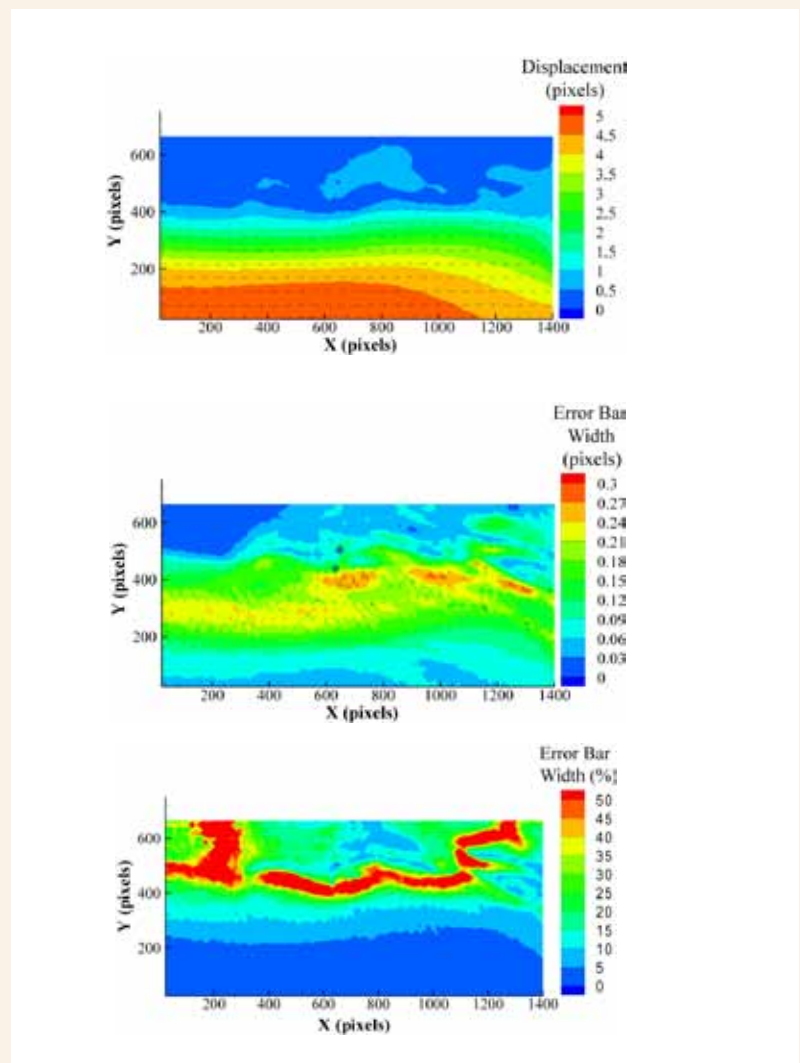


**Top to bottom: velocity, uncertainty , and relative uncertainty fields from particle image velocimetry experiment on a laminar separation bubble using software developed in this project.**

# Stardust: From Solar System Origins to National Security Applications

*An LLNL team is sampling and analyzing the building blocks of the solar system*



Artist's conception of the Stardust spacecraft approaching Comet Wild 2. The particle collector, filled with lightweight aerogel glass foam, is shown extended upward. The spacecraft is flanked by two solar panels. (Image courtesy of  NASA).

Stardust, the first U.S. solid-sample space mission since 1973's Apollo 17, returned the first materials ever collected from a known comet. With LDRD support, an LLNL team is developing the capabilities to capture cometary and interstellar dust particles, extract those particles from the aerogel collection foam, and determine the particles' makeup. The samples, from the comet Wild 2, are a time capsule containing material from the Solar System when it first formed.

*" . . . some of the most significant information . . . is at the atomic scale."*

## Why It Matters

Extraction and analysis technology developed by several Livermore LDRD projects for the Stardust mission is crucial for obtaining the maximum possible information from the relatively small amounts of materials that such next-generation space missions will return to Earth. Analysis shows that Comet Wild 2 contains an impressive assortment of materials, many unexpected. In particular, the comet contains an abundance of high-temperature minerals that appear to have formed in the inner regions of the solar nebula, which strongly suggests that the formation of the solar system included mixing over radial distances much greater than has been generally accepted by scientists.

## Methods

Livermore played a major role in developing particle extraction technologies adopted by the National Aeronautics and Space Administration. At the Johnson Space Center, team members assisted in some of the first extractions using a tiny knife developed by Hope Ishii, an LDRD researcher and materials scientist. The knife has a diamond blade that vibrates at ultrasonic frequency to make smooth cuts in aerogel, a difficult task because the brittle material is prone to breaking. The ultrasonic knife is one of several aerogel cutting tools developed to extract cometary particles at the center.

Livermore scientists are characterizing particles extracted from both aerogel and collector foil by developing

capabilities with highly specialized instruments such as the super scanning transmission electron microscope (SuperSTEM), nanometer-scale secondary-ion mass spectrometer, scanning electron microscope, and nuclear microprobe. SuperSTEM allows atomic-scale analyses of a particle's composition and produces stunning pictures magnified several million times. The machine has ancillary equipment that corrects images for blurring, yielding striking images of a mineral's crystalline structure. "SuperSTEM is invaluable because some of the most significant information contained in the Stardust samples is at the atomic scale," says John Bradley, who heads the Livermore team.



**Materials scientist Hope Ishii (right) exhibits a sample of aerogel containing cometary particles. The plastic barrier protects from contamination.**

## What's Next

The extraction techniques being developed can be applied to fusion-class laser experiments in support of Stockpile Stewardship and energy research, seeking to recover, from aerogel, particulate ejecta generated during laser shots. The Stardust team's integrated analysis approach also has application to the interrogation of nuclear materials in nuclear forensic studies supporting national security objectives. When the spacecraft was launched in 2004, many of the analytic techniques being used to examine Wild 2 particles didn't exist. "We expect new techniques to come along over the next few years that will provide important additional information," Bradley says. As data accumulate, the results will permit a thorough comparison with samples from asteroids, believed to have been formed in the warmer, inner regions of the solar system, and with interplanetary dust collected from Earth's stratosphere.

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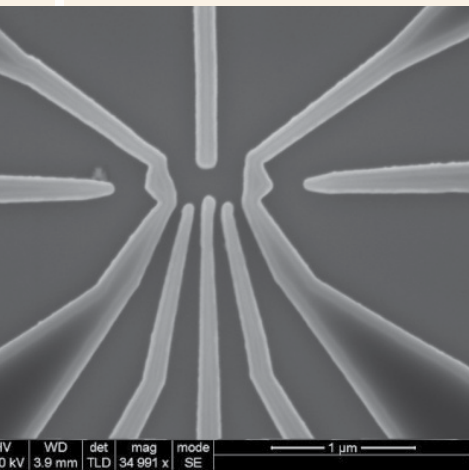
## Acknowledgments

# Computational Power from Spinning Electrons

## *Quantum Computing Will Solve Problems too Complex for Classical Computers*



**Electron micrograph of the fabricated silicon electrostatic electron-confinement chamber.**

Quantum computers offer a means of solving certain types of problems that are currently intractable for even the most powerful classical computers. Engineering the essential elements of a quantum computer—quantum bits (qubits)—requires isolation of either a single ion (ion trap) or a single or few electrons. Achieving this feat in silicon is a more-daunting challenge than previous work in other materials, but also has great advantages. This project has been successful at electrostatically isolating single or few electrons in silicon quantum dots, thereby creating qubits that can be more-readily integrated with the silicon-based semiconductor circuitry that forms the basis for much of modern electronics. This is critical because quantum computers are meant to supplement rather than supplant classical computers. The project has also designed such supporting electronics—designed to function cryogenically. Computational modeling of the design for a few-electron system has also been an outcome, as has the design of a "logical qubit," one that incorporates error correction algorithms adding fault tolerance. "This project's risk entailed going from zero to world-class in three years," noted Sandia principal investigator," Malcolm Carroll. "The effort is consistent with the best kind of work that is expected from a DOE national laboratory," noted the project's external advisory board.

## Why It Matters

Quantum computing exploits the unique quantum properties of superposition, entanglement, and interference to efficiently compute solutions that are classically difficult to solve. Examples include factoring (which is the basis for many of today's public key cryptosystems), unstructured search (e.g., given a phone number, find the owner in a phone book that is sorted by name), and precision simulation of complex quantum systems (useful for understanding the quantum properties of materials). These problems have national security applications that are of interest to DOE, DoD, and DHS.

## Methods

While current computers encode information as a sequence of discrete (noninteracting) bits, each of which occupies the alternative states of one or zero, a qubit — encoding information using electron spin — has the property of superposition, that is, of existing in a combination of one and zero states. Additionally, qubits can be interactively entangled, that is, one can influence the state of another. Hence, the encoding of information by a succession of qubits is far richer in possibilities than encoding by classical (one-zero) bits. Problematically, electron spin is a transient property, its "decoherence time" — the interval before loss of information —longer for silicon than for other materials. Fabrication of silicon electrostatic electron-confinement chambers and cryogenic circuitry

made use of Sandia's CMOS (complementary metal oxide semiconductor) technology at its Microsystems and Engineering Sciences Application (MESA) facility.

## What's Next

Follow-on activities include completion of next-generation cryogenic electronics, pursuit of silicon-germanium qubits (SiGe) as possibly superior to silicon, as well as ongoing parallel trapped-ion approaches to qubit fabrication. LDRD has supported both the quantum dot and trapped-ion approaches. Samples have been supplied to outside users in the quantum computation community (National Institute of Standards and Technology [NIST], Princeton University, and Lawrence Berkeley National Laboratory [LBNL]), and one of the project's team members serves on the external advisory board of the Australian Centre for Quantum Computing (University of Melbourne).  There are numerous other university collaborators.

*"This project's risk entailed going from zero to world-class in three years."*



**Modeled electron density in the electrostatic electron-confinement chamber.**

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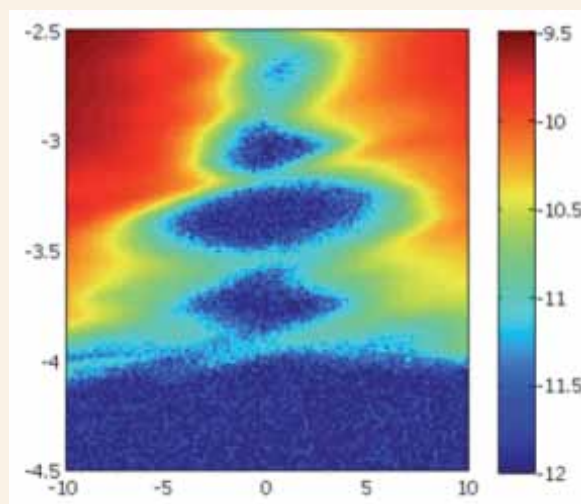
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## Acknowledgments
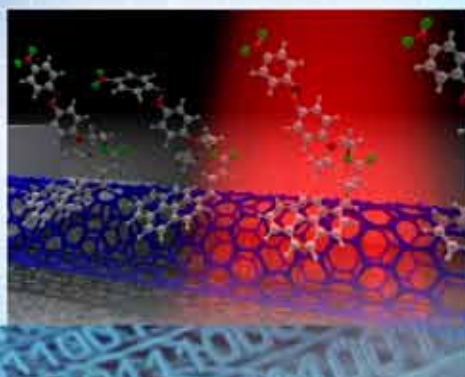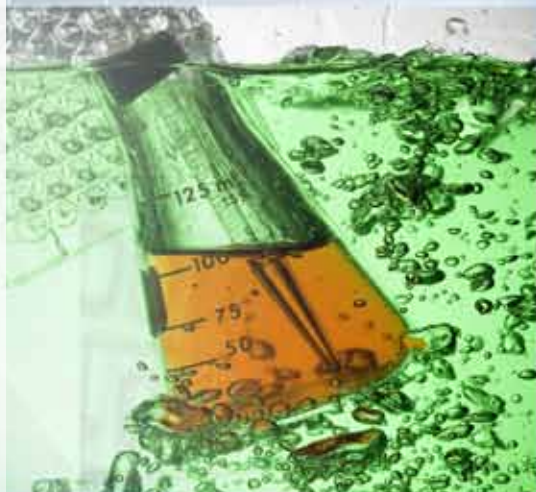
# Scientific Innovation and Discovery

Within the LDRD program, DOE scientists investigate fundamental aspects of the constituents and properties of matter at the nano-, micro-, and macro-scale, including the properties of complex materials, and those of biological systems.  In extending the understanding of nature, such research, in turn, enables new technologies that support  the energy, environment and nuclear security missions.  Scientific discovery feeds technology, and advanced technologies enable scientists to pursue more challenging aspects of research into fundamental phenomena.  LDRD scientists  pursue such research at the leading edge, investigating  topics such as quantum computing and more energy-efficient computation, high-temperature superconductivity, novel photovoltaic and nanomaterials, biocompatible materials for drug delivery, bio-inspired (and other) solutions to improved cyber security, and new detector technologies for studying both the smallest interactions of matter at the nanoscale and at the vast expanse of the universe.

In all these examples, LDRD scientists lead the way into new science, technology, and engineering (ST&E) territory, paving the path for solutions and innovations that anticipate the science and technology the Nation will require to remain competitive on the world stage and to also respond to technological surprises.

# Rapid Differential Diagnosis of Patients and Bioweapons

## ANL's Diagnostic Biochip

### Results

Argonne researcher Dan Schabacker has developed diagnostic biochips that are dual-use with applications in medical as well as in biosecurity fields. They can diagnose either infectious diseases or cancers, especially when patients present with ambiguous symptoms. The biochip can be used to identify biomarkers for the deadly drug-resistant MRSA (Multiply resistant *Staphylococcus aureus*) bacteria, for example, or—in collaboration with University of Chicago liver oncologists—a particular liver cancer marker that appears before the cancer is clinically detectable. The same ability to identify disease markers makes the chips useful for identifying bioweapons.

### Why It Matters

The chips offer doctors both the ability to quickly diagnose patients, and also, to give counterterrorism officials a new tool to hunt down manufacturers of biological weapons.

In this latter context, the biochips can be used to track protein "fingerprints" of biological weapons, yielding information that is capable of discerning where the microbes were grown and handled. For example, anthrax proteins differ according to the conditions under which the *B. anthracis* bacteria were grown; tracking these proteins reveals information about the skills and resources of the operator. Termed "microbial forensics," this science helps counterterrorism agencies find perpetrators and build a solid legal case.

"The ultimate goal is to build a library of 'signatures' of anthrax bacteria grown and prepared under various conditions, which can be used to identify an unknown sample from a possible terrorist attack," Schabacker said.

### Methods

Developed partially with LDRD funding earlier this decade, a biochip consists of a tiny array that contains anywhere between several dozen and several hundred "dots," or small drops. Each of these drops contains a unique protein, antibody or nucleic acid that will attach to a particular reagent. These proteins are collected from the pathogen or cancerous site and separated with a process called fractionation.

Researchers use different chemicals, or reagents, to characterize the resulting biochips, just as a detective would dust for fingerprints. When a reagent interacts with a particular protein fraction, that spot will "light up," creating part of the protein signature. Different combinations of spots create a unique "fingerprint" for each pathogen or cell under evaluation that can be read with automated equipment.

### What's Next

Argonne licensed the biochip technology to a firm in Frederick, Maryland to make the technology widely available. It has focused on identifying clinical pathogens, particularly tuberculosis and MRSA, that could be diagnosed with the biochip—creating a device that could be useful in any doctor's office across the country. The product is currently in FDA trials.

**Argonne biologist Dan Schabacker loads a biochip onto a reader for analysis.**

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*"The ultimate goal is to build a library of 'signatures' of anthrax bacteria . . . which can be used to identify an unknown sample from a possible terrorist attack."*

# From Brains to Baggage: A New Take on MRI

## LANL's MagViz opens new possibilities for MRI applications



**Top: A typical bin containing various liquid containers. Bottom: MagViz scan—Hazards are indicated by red dots while safe liquids are indicated in green.**

Thanks to a team of Los Alamos researchers, an innovation originally intended to take pictures of the brain can now enhance airport security. About two years ago, an interdisciplinary team of researchers and students coaxed brain images from a new, ultralow-field MRI system. Instead of the powerful magnet used in traditional MRI, the Los Alamos device uses an ultralow-field magnet similar in strength to the magnetic pull of the Earth—about 46 microteslas. By contrast, hospital MRI machines create a magnetic field 10,000 to 100,000 times Earth's magnetic field.

In the process of developing the brain scanner, Bob Kraus and his team seized upon the idea that a versatile, low-field MRI might have applications beyond just medicine. The researchers hypothesized that they might be able to distinguish different liquids. The team found the system to be remarkably discriminating. "If we can tell the difference between V8 juice and Coca Cola, which are mostly water," Kraus said, "why can't we tell the difference between shampoo and a threat substance?" The world's most sensitive magnetic field detector could be used to screen carry-on liquids at airports.

## Why It Matters

Having liquids on airplanes has been an issue in air travel security since measures were implemented in 2006 to address the threat of terrorists using liquid explosives onboard aircraft. Although traditional MRI machines could detect the slightly different chemical signals of the hydrogen atoms in liquids such as shampoo from those in liquid explosives, such machines have numerous drawbacks for application to airport security, beyond size and cost. Traditional hospital MRI machines depend on huge superconducting magnets that draw strong signals from scanned objects and provide clear resolution in the final images, allowing diagnosis of a torn knee ligament or a malignant brain tumor. However, because of the strong magnet, any metal present muddies the signal and creates unusable images, so shuttling metal-containing suitcases, and laptops, through an MRI security line at the airport would be impossible.

## Methods

In an MRI machine, magnetic fields cause hydrogen atoms to line up and spin in a substance placed within its field. Kraus likens this to toy tops spinning on a table in synchronization with each other. Eventually, the tops begin to wobble, falling out of rhythm. This wobbling of hydrogen atoms occurs in unique patterns for different chemicals. Sensors in the machine detect these slightly different frequencies, in effect, chemical fingerprints.

The fainter signals that MagViz teases out with a weaker magnet challenged the Los Alamos team to make sense of the less-distinct images. To increase the strength of the signal, the team incorporated a prepolarization field 100 times stronger than the magnet used to measure the spin. The technology relies on sophisticated detectors called superconducting quantum interference devices, or SQUIDs. Whereas

a hospital MRI detects spin with a sensor akin to a radio antenna, tuned to a specific set of frequencies, SQUIDs can pick up the oscillation of hydrogen or other atoms at any frequency.

Such sensitivity causes SQUIDs to receive both the desired signal and also significant noise — unwanted information. So the MagViz team has engineered new ways of filtering out the unwanted background noise. "The new generation of SQUIDs has an exquisite signal-to-noise ratio," Kraus explains.  Another hurdle involved the superconductors in SQUIDs, which require supercooling with liquid helium down to 4 Kelvin (–269 degrees Celsius). The $20,000 helium-chilled cryostat is the most expensive component of the system, and the MagViz team is working on ways to recycle the helium and use it more efficiently.

Linked with a computer database, MagViz can now reliably identify some 50 liquids from their chemical fingerprints. If MagViz finds a chemical designated as a threat, the machine will mark the container with a red dot on the screen. Harmless substances get a green dot, and if the machine can't identify the liquid, a yellow dot appears, indicating that further inspection is needed. As new threats emerge, they will be added to the database and the "gate" set. That gate is a tunable security threshold that can be set very stringently, so that only the most benign substances get the green designation. Or, the tolerance can be relaxed to allow more liquids through and increase the speed of baggage screening. In its current incarnation, MagViz takes about a minute for the whole process.

## What's Next
The Homeland Security Advanced Research Project Agency (HSARPA) at the U.S. Department of Homeland Security Science and Technology Directorate, which is supporting this project with a $5 million

## " . . . tell the difference between shampoo and a threat substance."

grant, hopes the final version will be able to scan bags at a speed similar to the current security checkpoint x-ray machines. The collaboration has also led to new ideas on how to further put ultralow-field MRI technology to use. The team envisions more portable (and less expensive) units, weighing just a few hundred pounds, that could be used by military medics for quick battlefield diagnostics or in hospitals in the developing world.

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**Bottles containing liquids about to pass, on a conveyor belt, into the heart of MagViz, an ultralow-field MRI machine developed for use at airport security portals.**

# Multifunctional Nanostructural Anti-corrosion / Anti-biofouling Coatings

*ORNL's superhydrophobic surface blocks growth of microorganisms on boats, submarines, underwater equipment*

A proprietary superhydrophobic coating could dramatically mitigate a multibillion dollar problem that affects underwater machines, watercraft, submarines, water intakes, offshore drilling rigs, and countless other types of equipment and machinery. Corrosion and biofouling costs the government and private sector upward of $276 billion, according to the National Association of Corrosion Engineers. The ORNL superhydrophobic surface can be used for a variety of metal, plastic and wooden surfaces and can significantly reduce the costs of maintenance and restoration of materials exposed to corrosive environments. While researchers plan to perform additional durability tests, results obtained in harsh conditions over four months are encouraging.

## Why It Matters

Given the magnitude of the problem caused by corrosion and biofouling, any substantial reduction in these areas would greatly increase a surface's lifetime, overall effectiveness and efficiency. ORNL's superhydrophobic silica-based coatings and deposition methods provide unprecedented protection, thereby substantially increasing the life of equipment while lowering maintenance costs.

## Methods

The "wettability" of a surface is determined by the water-surface interactions and the surface roughness. The team, led by John Simpson, was able to change the wettability state by tailoring the surface topology and surface chemistry. The resulting structures consist of an outer layer of nanotextured sand with dimensions ranging from tens of nanometers to a few microns.

*" . . . substantially increasing the life of equipment while lowering maintenance costs."*
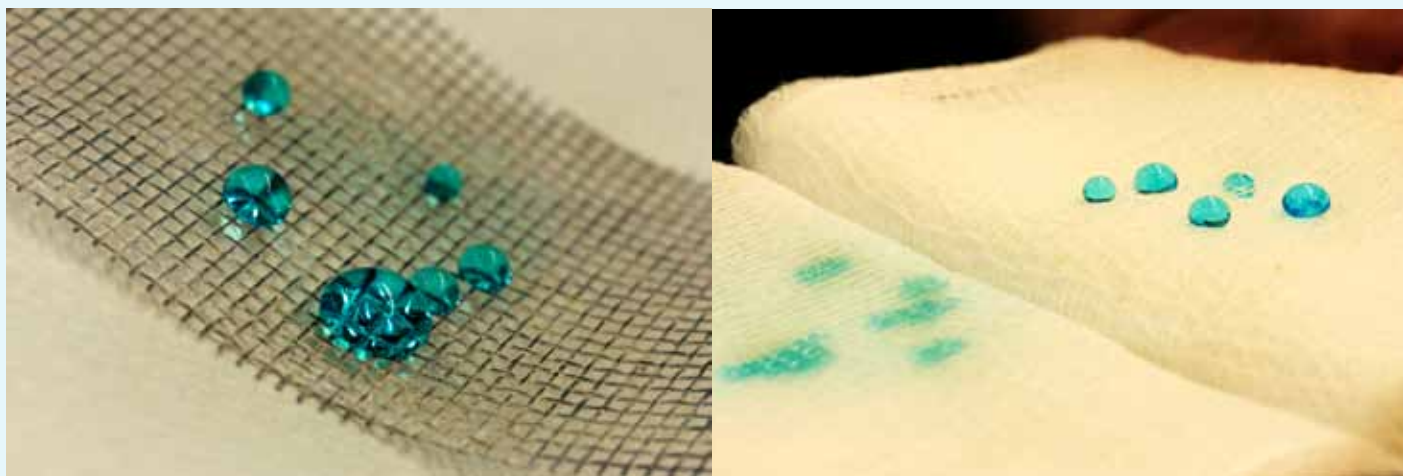
**Illustration of the beading of colored water droplets on surfaces coated with the process: left, metal screening; right, fabric.**

The technology is based on superhydrophobic nanotextured silica (sand) bonded to a variety of surfaces using organic binders consisting of silicone oil and polymers dissolved in solvents. The polymers provide an adhesion layer that enables the superhydrophobic particles to form a nano- to microstructured anti-biofouling and anti-corrosion surface, whereas the silicone oil enhances the properties of the coating. The nanostructured surface combined with a silicone oil layer blocks microorganism adhesion.

The silicone oil plays a significant role in the properties of the coating. It is inert, incompressible, and practically insoluble in water. In addition, the silicone oil–modified superhydrophobic surface appears and feels dry.

## What's Next
Durability testing continues as the technology is being evaluated for marine coatings for the U.S. Navy and other military uses. In addition, the technology was recently licensed to Veloxflow, a start-up that will initially use the technology to coat municipal water system piping. Veloxflow has plans for other uses.

Clothing and fabric manufacturers for military and non-military applications have expressed interest, as have representatives in the building materials industry.

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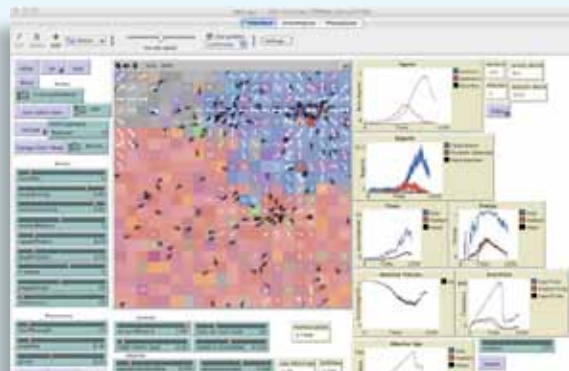
# Digital Ants—One of Ten World Changing Ideas

*PNNL develops digital ants that wander through computers searching out then swarming viruses and worms*

**Tiny programs are modeled on real ant behavior. The programs "wander" through computers searching out and then swarming viruses and worm.**

The Pentagon's computers experience more than five thousand attacks every day. Large, shared computer networks need a secure defense system to protect against adversaries. The current defensive methodology gathers all cyber threat data from across the various points within an organization and funnels it into a queue to a single point for analysis. It can take days or weeks for the solutions derived from these analyses to be implemented. By that time, a cyber attack may have spread or changed form.



**PNNL computer scientists led by Dr. Glenn Fink and researchers at Wake Forest University developed a new type of computer network security software modeled after ants.**

To address this challenge, PNNL researchers, in collaboration with scientists from Wake Forest University, have developed Digital Ants that roam a computer network looking for perceived threats—similar to how real ants protect a nest. Cited as one of 10 innovative technologies in *Scientific American*, Digital Ants is a framework for decentralized coordination based a social behavior in ant colonies known as "swarm intelligence."

## Why It Matters

In the never-ending battle to protect computer networks from intruders, security experts are deploying new defenses. Every computer attack is a battle between the owners of a computational infrastructure and adversaries bent on using these resources for their own purposes. The problem of securing complex infrastructures in a dynamic hostile environment with changing adversaries cannot be solved with static defenses or uncoordinated unilateral measures. Unlike traditional security devices, Digital Ants wander through computer networks looking for threats, such as computer worms—self-replicating programs designed to steal information or facilitate unauthorized use of machines. When a Digital Ant detects a threat, it doesn't take long for an army of ants to converge at that location, drawing the attention of human operators who step in to investigate. The concept—known as swarm intelligence—promises to transform cyber security because it adapts readily to changing threats.

## Methods

In today's large infrastructures, the way we typically monitor cyber defense is to gather all the cyber data from across the enterprise to a single point and analyze it centrally. While this gives an excellent scope of information, this approach scales poorly. To address this challenge, Glenn Fink, a PNNL

*"Ants defend themselves against threats very successfully . . . achieve that . . . in a computer system."*

research scientist, came up with the idea of copying ant behavior. "In nature, we know that ants defend themselves against threats very successfully," Wake Forest Professor of Computer Science Errin Fulp, an expert in security and computer networks, added. "They can ramp up their defense rapidly, and then resume routine behavior quickly after an intruder has been stopped. We were trying to achieve that same framework in a computer system."

As the ants move about the network, they leave digital trails modeled after the scent trails ants in nature use to guide other ants. Each time a digital ant identifies some evidence, it is programmed to leave behind an evaporating digital "scent trail." Stronger scent trails attract more ants, producing the swarm that marks a potential computer infection. When the problem is solved, the evidence goes away and the scent trails disappear.

The new security approach is best suited to protect a large network of networks each owned and operated by separate enterprises or agencies. Networks like those used to connect the emerging smart power grid are ideal candidates for digital ants. And computer users need not worry that a swarm of digital ants will decide to take up residence in their machine by mistake. Digital ants cannot survive without software "sentinels" located at each machine, which in turn report to network "sergeants," monitored by humans who supervise the colony and maintain ultimate control. "Rather than taking humans completely 'out of the loop,' we want to place human operators in the *right loop*, where they can supervise while letting the ants do most of the work," said Fink.

## What's Next

This project is currently investigating ways to employ digital ants to protect smart electric grid for DOE's Cybersecurity for Electric Distribution Systems project, and cloud computing to protect NSF's Global

Environment for Network Innovations (GENI) network. Digital Ants will protect the numerous new smart grid devices in homes and industry from Internet-borne attacks. In the GENI cloud, Digital Ants will help prevent malicious users from harming other users or the underlying hardware and software of the cloud.

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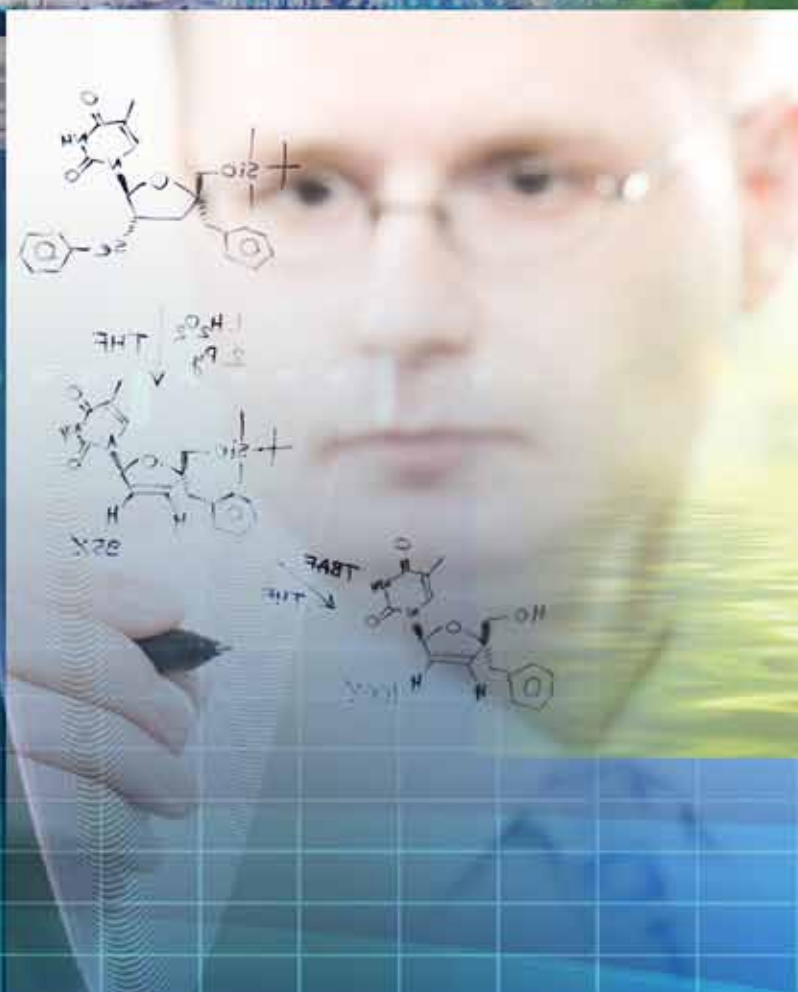
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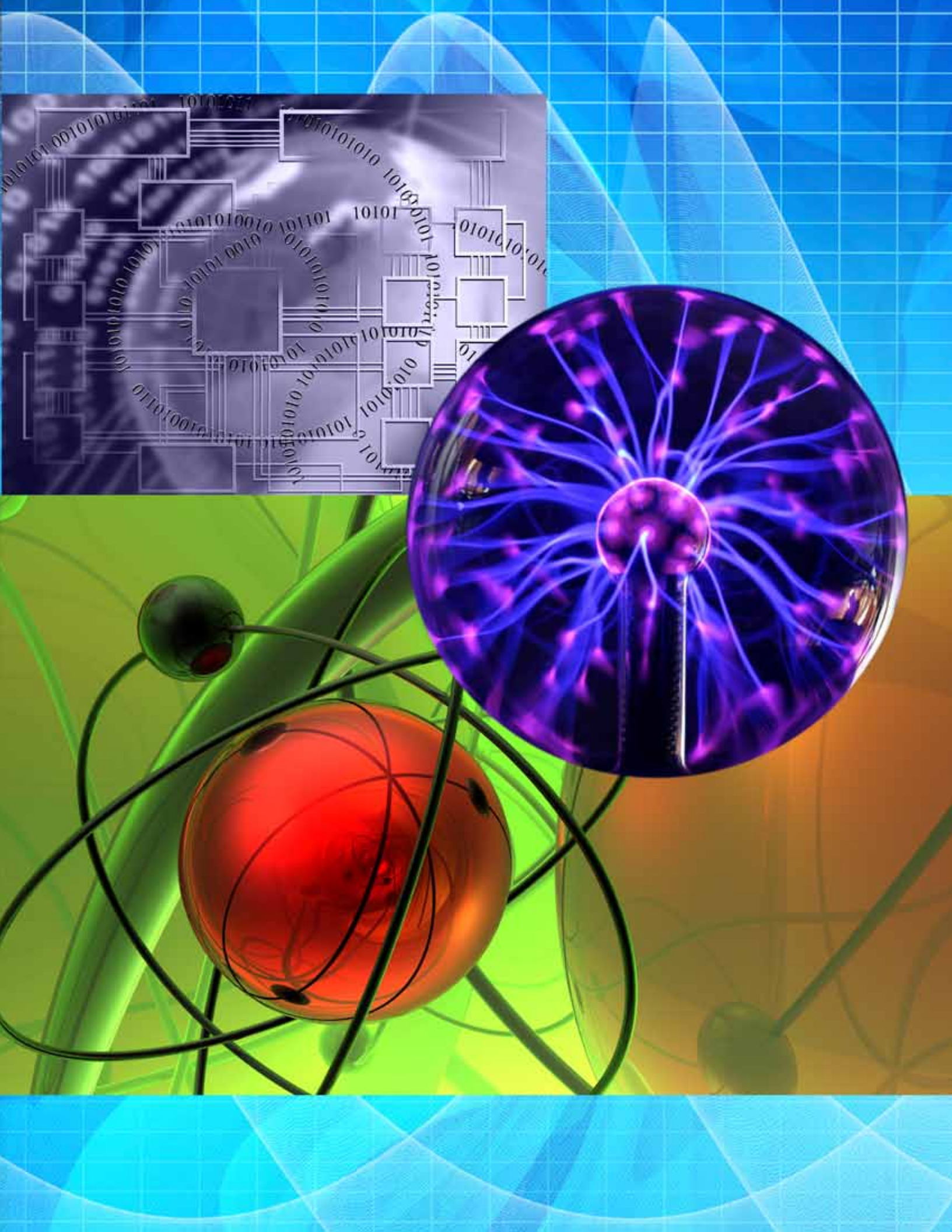
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## Acknowledgements

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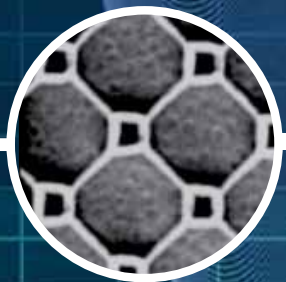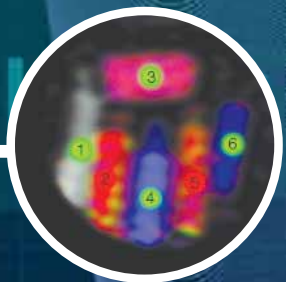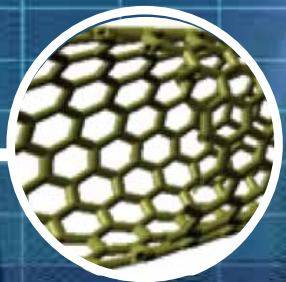Washington, DC  80585
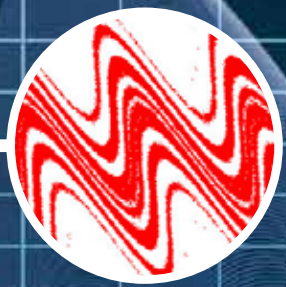jamileh.mogin@nnsa.doe.gov
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